

Simulating Bosonic Baths with Error Bars

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We derive rigorous truncation-error bounds for the spin-boson model and its generalizations to arbitrary quantum systems interacting with bosonic baths. For the numerical simulation of such baths the truncation of both, the number of modes and the local Hilbert-space dimensions is necessary. We derive super-exponential Lieb–Robinson-type bounds on the error when restricting the bath to finitely-many modes and show how the error introduced by truncating the local Hilbert spaces may be efficiently monitored numerically. In this way we give error bounds for approximating the infinite system by a finite-dimensional one. As a consequence, numerical simulations such as the time-evolving density with orthogonal polynomials algorithm (TEDOPA) now allow for the fully certified treatment of the system-environment interaction.

Introduction – Ideal quantum systems may be considered closed, undergoing textbook unitary evolution. In any realistic experimental setup however a quantum system is open, that is, it interacts with an environment composed of those degrees of freedom that are not under the control of the experimenter. Hence the numerical and analytical description of the dynamics of a quantum system in interaction with its environment is of fundamental importance in quantum physics. The precise nature and composition of the system-environment interaction is generally not known, but for a wide range of systems encountered in physics, chemistry, and biology, it is common to model the environment as a continuum of harmonic oscillators, which interact linearly with the system. This results in the paradigmatic spin-boson model that captures many aspects of the system-environment interaction [1]. The spin-boson model is exactly solvable only in the rarest of special cases and one is therefore compelled to employ a variety of approximations and numerical descriptions in order to obtain the reduced dynamics of the quantum system in question. Notable examples include those cases in which the environment possesses a correlation time that is much shorter than the system dynamics *and* the system-environment interaction is weak. Under these assumptions it is then well-justified and customary to resort to the so-called Markov approximation which permits the derivation of completely positive and linear differential equations, the Lindblad equation, for the quantum system alone [2].

However, settings of considerable practical importance may violate either or both of these assumptions and require a more sophisticated treatment. The recently emerging interest in quantum effects in biological systems provides a case in point [3]. For instance, in typical pigment-protein complexes the dynamical time-scales of the vibrational environment can be comparable or even slower than the quantum mechanical excitation energy transfer dynamics. Moreover, in the limit of slow bath dynamics, perturbative treatments of the coupling between system and environment cannot be used even if the system-bath coupling is intrinsically weak. Consequently, steps have been taken towards the development of

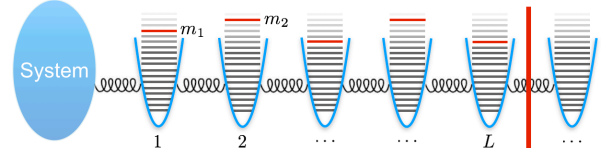


FIG. 1. A system coupled to a bosonic bath. Red lines indicate the truncations: The spatial truncation to a chain of finite length L and the truncation of the local Hilbert space dimensions to m_i .

non-perturbative and non-Markovian approaches for the description of the quantum system-environment interaction (see [3, 4] for overviews of recent developments). However, the majority of these approaches have in common that they exploit approximations that are not well controlled in the sense that no rigorous error bounds on the simulation results are available. Hence these methods are not certified.

The time evolving density with orthogonal polynomials algorithm (TEDOPA) for the spin-boson model presents a notable exception, as will be demonstrated in the present work. It makes use of an exact transformation of the standard representation of the spin-boson model onto a spin interacting with the first site of a semi-infinite nearest-neighbor coupled chain [5–9] which renders the system particularly amenable to time-adaptive density matrix renormalisation group (t-DMRG) simulations. The structure of the resulting system is such that excitations tend to propagate along the chain away from the system towards infinity leading to irreversible system dynamics for long times. This approach has been used with success in the simulation of a number of highly non-Markovian system-environment interactions [6, 10, 11].

The errors that accumulate in the t-DMRG simulation can be bounded rigorously. Nevertheless, the numerical TEDOPA simulation employs two as yet uncertified assumptions: (i) the semi-infinite chain needs to be truncated to a finite length and (ii) the local dimension associated with each harmonic oscillator of the chain the needs to be truncated to a finite dimensional Hilbert space, see Fig. 1. The errors that are introduced in this manner are usually estimated by increasing both the chain length and Hilbert space cut-off until the change in the result drops below a predefined threshold. However, in practice this somewhat inelegant approach can become highly

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challenging numerically, and can lead to erroneous numerical predictions [12]. A more rigorous approach is therefore desirable.

Here we employ techniques that lead to Lieb–Robinson type bounds to achieve this goal by deriving bounds for the errors arising from approximations (i) and (ii). As the errors arising in each step of the t-DMRG integration can also be bounded we arrive at a method that possesses rigorous error bounds on the results that it delivers. This extends significantly existing recent results in the literature that apply to the finite dimensional setting of spin systems [13] and therefore allows the fully certified treatment of the system–environment interaction for both, harmonic oscillator as well as spin environments.

The system under consideration – We will consider the Hamiltonian of an arbitrary system \hat{H}_S coupled via \hat{V} to a bosonic bath described by \hat{H}_B so that the total Hamiltonian reads

$$\hat{H} = \hat{H}_S + \hat{V} + \hat{H}_B. \quad (1)$$

For simplicity and to directly connect to the TEDOPA approach [6, 7, 10, 11], we assume that \hat{H}_B describes a one-dimensional nearest-neighbour Hamiltonian (the higher dimensional case with more general couplings will be published elsewhere [14]) and takes the form

$$\hat{H}_B = \frac{1}{2} \sum_{i,j=0}^{\infty} (\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j), \quad (2)$$

where we assume that only nearest-neighbours are coupled, $X_{i,j} = P_{i,j} = 0$ for $|i - j| > 1$, and we let w.l.o.g. $X_{i,j} = X_{j,i} \in \mathbb{R}$, $P_{i,j} = P_{j,i} \in \mathbb{R}$. We consider system–bath couplings of the form $\hat{V} = \hat{h} \otimes \hat{x}_0$ (see the appendix for systems coupled to several baths), where \hat{h} acts on the system and we assume that it is bounded in operator norm, $\|\hat{h}\| < \infty$. The system with Hamiltonian \hat{H}_S has no restrictions, it can correspond to any system—bosons, fermions, and/or spins, all in arbitrary dimensions.

Spatial truncation of the bath – For bounded system observables \hat{O} , $\|\hat{O}\| < \infty$, We are interested in the quantity

$$\Delta(t, L) = |\text{tr}[\hat{O} e^{-i\hat{H}t} \hat{\rho}_0 e^{i\hat{H}t}] - \text{tr}[\hat{O} e^{-i\hat{H}_L t} \hat{\rho}_0 e^{i\hat{H}_L t}]|, \quad (3)$$

i.e., the error introduced when, instead of simulating the full Hamiltonian \hat{H} , we simulate the time evolution of system observables \hat{O} with the truncated bath Hamiltonian

$$\hat{H}_B^L = \frac{1}{2} \sum_{i,j=0}^{L-1} (\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j) \quad (4)$$

and corresponding total Hamiltonian $\hat{H}_L = \hat{H}_S + \hat{V} + \hat{H}_B^L$. Our first main result is the following.

Theorem 1 *Let \hat{H} and \hat{H}_L be as above. Let $X, P > 0$ or $X = P$ (see the appendix for a bound when neither of these*

conditions is satisfied). Let c be such that $\|XP\|^{1/2} \leq c$. Then

$$\frac{\Delta^2(t, L)}{4\|\hat{O}\|^2\|\hat{h}\|/c} \leq C \left(\|\gamma_0\|^{1/2} + t\|\hat{h}\| \right) \frac{(ct)^{L+1}(e^{ct} + 1)}{(L+1)!}, \quad (5)$$

where $C = \|P_L\| \|X_{L-1,L}\|/c^2 + \|P_{L-1,L}\|/c$ and

$$\gamma_0 = \begin{pmatrix} \gamma_{xx} & \gamma_{xp} \\ \gamma_{px} & \gamma_{pp} \end{pmatrix}, \quad [\gamma_{ab}]_{i,j} = \text{tr}[\hat{a}_i \hat{b}_j \hat{\rho}_0], \quad (6)$$

collects the two-point bath correlations in the initial state. If $P \propto \mathbb{1}$, we may replace L by $2L$ in Eq. (5).

If the initial 2-point correlation functions (the matrix elements of γ_0) are unbounded, then one can still achieve bounds, see the appendix for details. The r.h.s. of Eq. (5) describes the Lieb–Robinson-type light cone [15]. Outside the light cone, so for $\tau := ect < L$, one finds super-exponential decay in L : $(ct)^L e^{ct}/L! \leq e^{ct-L} |\ln(L/\tau)|$. This makes rigorous the physical intuition that for all finite times only a chain of *finite* length is required to simulate the dynamics of local observables to within a prescribed precision. Our bound applies to *any* system Hamiltonian, unbounded or otherwise, and depends only linearly on the operator norm of the system coupling $\|\hat{h}\|$. The proof relies on Lieb–Robinson bounds for harmonic systems [16–18] (see also Ref. [19]) and may be found in the appendix. Before stating our second main result, we discuss the above bound in the light of the generalized spin-boson model.

Generalised spin-boson model – In this section we will investigate Hamiltonians of the form

$$\hat{H} = \hat{H}_S + \int d\mathbf{k} g(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \hat{A}_S \int d\mathbf{k} h(\mathbf{k}) (a_{\mathbf{k}}^\dagger + a_{\mathbf{k}}). \quad (7)$$

This describes a quantum system with Hamiltonian \hat{H}_S interaction with a bath of bosons; it is described in more detail in terms of second quantised operators in [20]. This model has received renewed interest in recent years due to its importance in the theoretical study of quantum effects in biology (see [3] for a review). An important quantity that describes the bath and its coupling to the system is the spectral density, which, for invertible g , is defined as

$$J(\omega) = \pi h^2 (g^{-1}(\omega)) \left| \frac{dg^{-1}(\omega)}{d\omega} \right|, \quad (8)$$

with g^{-1} the inverse of g . The smallest closed interval containing the support of g^{-1} is denoted $[\omega_{\min}, \omega_{\max}]$. The case $\omega_{\min} = 0$ is called massless where as $\omega_{\min} > 0$ is known as massive.

Building on the work of [5, 7, 8], it was shown using the theory of orthogonal polynomials in [9] that Eq. (7) can be written in the form of Eqs. (2,1) and that there are two ways to do this. Both choices

$$\hat{h} = \mu_0 \hat{A}_S, \quad X = P, \quad (9)$$

and

$$\hat{h} = \mu_1 \hat{A}_S, \quad P = \omega_{\max} \mathbb{1}, \quad (10)$$

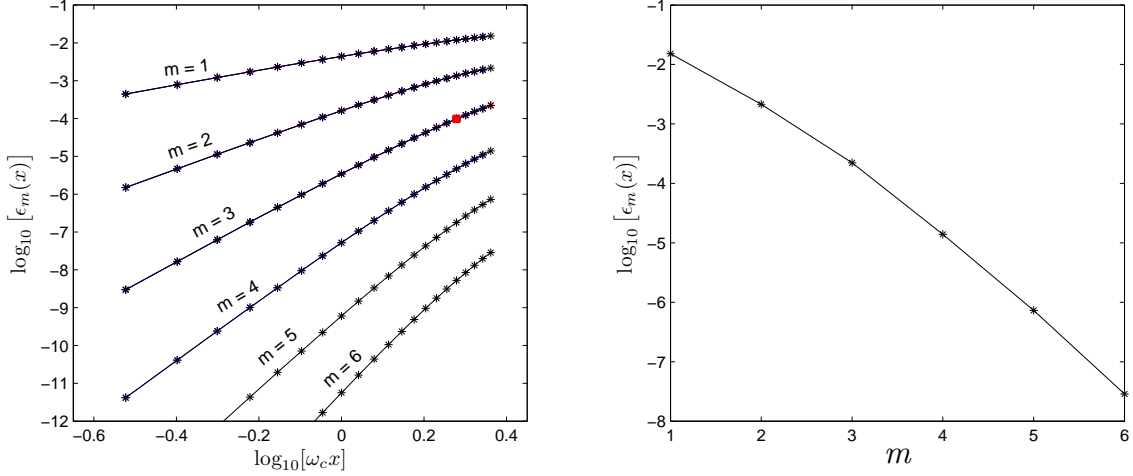


FIG. 2. Fock space truncation error (Eq. (17)) for the particle mapping and power-law spectral densities as in Eq. (19) with $\Delta/\omega_c = 1$, $\alpha = 0.8$, $s = 3$ for initial state $\hat{\rho}_0 = \hat{\rho}_S^0 \otimes \hat{\rho}_B^0$, $\hat{\rho}_S^0 = |\uparrow\rangle\langle\uparrow|$ and $\hat{\rho}_B^0$ the vacuum. We truncate each local Hilbert space at the same value $m_i = m$ and L has the values 3 to 6, but are indistinguishable (e.g. the difference between the $L = 6$ and $L = 3$ curve at the point denoted by a red square is 4.95×10^{-6}). Lines are guides to the eye. The log-log plot on the left suggest algebraic increase in time and the plot on the right suggests better than exponential decrease with m .

with appropriate X (given in terms of the spectral density in the appendix) are equivalent to Eq. (7). Here,

$$\mu_0^2 = \frac{2}{\pi} \int d\omega J(\omega), \quad \mu_1^2 = \frac{1}{\pi\omega_{max}} \int d\omega J(\sqrt{\omega}) \quad (11)$$

and one finds $\|X\| = \|P\| = \omega_{max}$ for both cases and $X > 0$ iff $\omega_{min} > 0$. Due to the form of their elementary excitations, the mappings leading to couplings as in Eqs. (9) and (10) were named *particle mapping* and *phonon mapping*, respectively, and we will adopt this denomination here. Crucially, in both cases, X couples nearest-neighbours only such that the bound in Eq. (5) is readily applicable to the particle and the massive phonon case, setting $c = \omega_{max}$ for both (similar results hold for the massless case, see appendix for full details). For the particle mapping, we find $C \leq 2$ and for the phonon mapping $C \leq 1$ such that, up to the constants $\mu_{0/1}$, we obtain the same behaviour of the bound in both cases but replacing L by $2L$ in the massive phonon case. Hence, for the phonon mapping with a chain of only half the length, one has approximately the same chain truncation error as for the particle mapping.

If the maximum frequency of the bath $\omega_{max} = \infty$, the chain coefficients are unbounded [9] and our bounds diverge. This divergence is not surprising in light of the observation that certain one-dimensional infinite harmonic lattice models with nearest neighbour interactions and unbounded coefficients have been proven *not* to have a light cone bound [22]. It is noteworthy, that similar results can be derived for the case of a fermionic bath, since the chain mapping is still valid and Lieb–Robinson bounds for fermions are well-known [23].

Truncating local Hilbert spaces – We now consider the error introduced when the local Hilbert space dimensions of the harmonic oscillators making up the bath are truncated. To this

end, we define the projector

$$\mathbb{1}_m = \mathbb{1}_{m_0} \otimes \cdots \otimes \mathbb{1}_{m_{L-1}}, \quad \mathbb{1}_m = \sum_{n=0}^m |n\rangle\langle n|, \quad (12)$$

where $\mathbb{1}_{m_i}$ acts on the i 'th site of the bath and truncates the local Hilbert space according to $\mathbb{1}_m$. For bounded observables acting on the system \hat{O} , $\|\hat{O}\| < \infty$, we consider

$$\Delta_m(t) = |\text{tr}[\hat{O}e^{-it\hat{H}}\hat{\rho}_0e^{it\hat{H}}] - \text{tr}[\hat{O}e^{-it\hat{H}_m}\hat{\rho}_0e^{it\hat{H}_m}]|, \quad (13)$$

i.e., the error introduced by evolving the system according to

$$\hat{H}_m = \mathbb{1}_m \hat{H} \mathbb{1}_m \quad (14)$$

instead of \hat{H} . Here, \hat{H} is as in Eq. (4) and we omit the index L for notational clarity. The truncated Hamiltonian reads $\hat{H}_m = \hat{H}_S + \hat{H}_B^m + \hat{h} \otimes \mathbb{1}_m \hat{x}_0 \mathbb{1}_m$, where

$$\hat{H}_B^m = \frac{1}{2} \sum_{i,j=0}^{L-1} [X_{i,j} \mathbb{1}_m \hat{x}_i \hat{x}_j \mathbb{1}_m + P_{i,j} \mathbb{1}_m \hat{p}_i \hat{p}_j \mathbb{1}_m]. \quad (15)$$

In the appendix we show that

$$\frac{\Delta_m^2(t)}{4\|\hat{O}\|^2} \leq \text{tr}[(\mathbb{1} - \mathbb{1}_m)\hat{\rho}_0] + 2 \int_0^t dx \sqrt{\epsilon_m(x)}, \quad (16)$$

where

$$\epsilon_m(x) = \text{tr}[\hat{h}^2 e^{-ix\hat{H}_B^m} \hat{X}^2(x) e^{ix\hat{H}_B^m} \hat{\rho}_m(x)], \quad (17)$$

with

$$\begin{aligned} \hat{X}(x) &= \mathbb{1}_m e^{ix\hat{H}_B} \hat{x}_0 e^{-ix\hat{H}_B} \mathbb{1}_m - e^{ix\hat{H}_B^m} \hat{x}_0 e^{-ix\hat{H}_B^m}, \\ \hat{\rho}_m(x) &= e^{-ix\hat{H}_m} \hat{\rho}_0 e^{ix\hat{H}_m}. \end{aligned} \quad (18)$$

Crucially, under the assumption that the system Hilbert space is finite dimensional, this error may be computed numerically as it involves only observables acting on the truncated Hilbert space ($e^{ix\hat{H}_B}\hat{x}_0e^{-ix\hat{H}_B}$ is a linear combination of the \hat{x}_i and \hat{p}_i) and which are of a form amenable to t-DMRG simulations (see the appendix for details). For all finite times, $\lim_{\{m_i\} \rightarrow \infty} \Delta_m = 0$ and we study its behaviour in m at the hand of numerical examples below. If the bath initially contains only a finite number of particles, $\text{tr}[(1 - 1_m)\hat{\rho}_0]$ vanishes for appropriate m . Such states include the vacuum state which is also the zero temperature thermal state for the particle mapping. For higher temperature thermal states of the bath, $\text{tr}[(1 - 1_m)\hat{\rho}_0]$ vanishes exponentially for large $\{m_i\}$. The total error induced on the expectation value of \hat{O} due to (i) truncating the chain to finite length and (ii) the truncation of the local dimensions is bounded by the sum of the two individual error bounds: $\Delta(t, L) + \Delta_m(t)$. This rigorously bounds the error of approximating an infinite-dimensional bath of bosons by a chain of length L made up of finite-dimensional subsystems with nearest neighbour interactions. If in addition we assume the system with Hamiltonian \hat{H}_S to be a spin system, then the Hamiltonian is in the class which, as [13] shows, can be simulated with resources polynomial in L and error ϵ , and exponential in $|t|$.

Numerical example – As an example, we consider the spin-boson model with power-law spectral density,

$$J(\omega) = \pi\alpha\omega_c^{1-s}\omega^s \Theta(1 - \omega/\omega_c), \quad (19)$$

where Θ is the Heaviside step function. This model has been extensively probed numerically, and there has been controversy over the accuracy of numerically derived critical exponents. One of the issues with the results was the inability to verify the local Fock space truncation errors [12, 24]. The system Hamiltonian and interaction part are $\hat{H}_S = -\Delta\hat{\sigma}_x/2$ and $\hat{A}_S = \sigma_z/2$. The dissipation is known as Ohmic for $s = 1$

and super ohmic for $s > 1$. This can be written in the chain representation using Eq. (9) (see the appendix for details). In Fig. 2, the bound for the particle mapping is plotted for the super-ohmic case and various L and m . Constants used for the simulation (see figure caption) are taken from the literature [21]. The initial state of the bath corresponds to the zero temperature thermal state. We probe the same initial state for the case of ohmic dissipation and achieve qualitatively the same results (see appendix). Furthermore, we test the bound for a squeezed vacuum state of the bath, which is a highly populated state (see appendix).

Conclusion – The detailed simulation of the interaction of a quantum system with a structured environments composed of harmonic oscillators has applications in a wide variety of scientific fields. The multitude of proposed algorithms to tackle this problem numerically lacked a method that delivers a simulation result with a rigorous error bound associated with it. In this work we derived error bounds that demonstrate that the recently developed TEDOPA can provide such a method. More specifically, obtaining Lieb–Robinson type expressions we provide complete error bounds on the simulation of observables of quantum systems coupled to a bosonic baths with infinitely many degrees of freedom such as the spin-boson model. This includes the errors incurred due to the truncation of the local Hilbert-spaces of the harmonic oscillators and due to the truncation of the length of the harmonic chain representing the environment. In this manner we provide a fully rigorous upper bound on the error for the numerical simulation of a spin-boson model and its generalisation to multiple baths and more general systems.

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Appendix A: Spatial truncation of the bath

We consider an arbitrary (not necessarily finite-dimensional) system described by a Hamiltonian \hat{H}_S and a bosonic bath described by

$$\hat{H}_B = \frac{1}{2} \sum_{i,j=0}^{\infty} [\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j], \quad (\text{A1})$$

where \hat{x}_i and \hat{p}_i are canonical position and momentum operators with the usual commutation relations $[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0$ and $[\hat{x}_i, \hat{p}_j] = i\delta_{i,j}$. As we are allowing the bath to consist of infinitely-many modes (infinitely-many lattice sites), we assume throughout that the domain of the Hamiltonian is well-defined. W.l.o.g., we let $X_{i,j} = X_{j,i} \in \mathbb{R}$ and $P_{i,j} = P_{j,i} \in \mathbb{R}$. We assume that they couple only nearest neighbours: $X_{i,j} = P_{i,j} = 0$ for $|i - j| > 1$.

We suppose that system and bath are coupled according to

$$\hat{V} = \hat{h} \hat{x}_0, \quad (\text{A2})$$

where \hat{h} acts on the system and we assume $\|\hat{h}\| < \infty$. Thus, our total Hamiltonian reads

$$\hat{H} = \hat{H}_S + \hat{V} + \hat{H}_B, \quad (\text{A3})$$

where for compactness of notation, we have neglected tensor products with the identity. We are interested in the error introduced for the time-evolution of bounded observables \hat{O} (assuming $\|\hat{O}\| < \infty$) acting on the system when, instead of simulating the full Hamiltonian \hat{H} , we take only finitely many lattice sites of the bath into account. Namely those that are closest to the site 0, truncating the bath Hamiltonian according to

$$\hat{H}_B^L = \frac{1}{2} \sum_{i,j=0}^{L-1} [\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j] = \frac{1}{2} \sum_{i,j} [\hat{x}_i (X_L)_{i,j} \hat{x}_j + \hat{p}_i (P_L)_{i,j} \hat{p}_j], \quad (\text{A4})$$

where X_L, P_L are the principle submatrices of X, P corresponding to the non-truncated modes. The truncated chain hence consists of L modes. Denoting the initial state of the whole system by $\hat{\rho}_0$ and the total truncated Hamiltonian by $\hat{H}_L = \hat{H}_S + \hat{V} + \hat{H}_B^L$, we set out to bound the difference

$$\Delta(t, L) = |\text{tr}[\hat{O} e^{-i\hat{H}t} \hat{\rho}_0 e^{i\hat{H}t}] - \text{tr}[\hat{O} e^{-i\hat{H}_L t} \hat{\rho}_0 e^{i\hat{H}_L t}]|. \quad (\text{A5})$$

We will prove the following theorem.

Theorem 2 (Spatial truncation of the bath) *Let \hat{H}, \hat{H}_L as above, c, c' such that $\|P_L X_L\|^{1/2} \leq c$ and $\max\{\|X\|, \|P\|\} \leq c'$. Then*

$$\Delta^2(t, L) \leq 4\|\hat{O}\|^2 \frac{\|\hat{h}\|}{c} \left(\frac{\|P_L\| \|X_{L-1,L}\|}{c^2} + \frac{|P_{L-1,L}|}{c} \right) \frac{(ct)^{L+1}}{(L+1)!} (e^{ct} + 1) \left(\|\gamma_0\|^{1/2} + \|\hat{h}\| \frac{e^{c't} - 1}{c'} \right) e^{c't}. \quad (\text{A6})$$

If $X, P > 0$ or $X = P$, we may take $c' \rightarrow 0$ such that we recover the theorem in the main text. If $P \propto \mathbb{1}$, we may replace $\frac{(ct)^{1+L}}{(L+1)!}$ by $\frac{(ct)^{2L+1}}{(2L+1)!}$. Here,

$$\gamma_0 = \begin{pmatrix} \gamma_{xx} & \gamma_{xp} \\ \gamma_{xp}^\dagger & \gamma_{pp} \end{pmatrix}, \quad [\gamma_{xx}]_{i,j} = \text{tr}[\hat{x}_i \hat{x}_j \hat{\rho}_0], \quad [\gamma_{pp}]_{i,j} = \text{tr}[\hat{p}_i \hat{p}_j \hat{\rho}_0], \quad [\gamma_{xp}]_{i,j} = \text{tr}[\hat{x}_i \hat{p}_j \hat{\rho}_0], \quad (\text{A7})$$

collects the two-point bath correlations in the initial state of the whole system. Note that $\|X_L\| \leq \|X\|$ and $\|P_L\| \leq \|P\|$.

One can allow for the two-point correlations collected in γ_0 to diverge and still get a bound on $\Delta(t, L)$, see Section A 1 c. Often, one encounters systems interacting with multiple baths. We generalize to this setting in Section A 1 d.

1. Proof

Denote

$$\hat{U}(t) = e^{it(\hat{H}-\hat{V})}e^{-it\hat{H}}, \quad \hat{U}_L(t) = e^{it(\hat{H}_L-\hat{V})}e^{-it\hat{H}_L}. \quad (\text{A8})$$

Then for system operators \hat{O}

$$\text{tr}[\hat{O}e^{-it\hat{H}}\hat{\rho}_0e^{it\hat{H}}] = \text{tr}[\hat{O}e^{-it(\hat{H}-\hat{V})}\hat{U}(t)\hat{\rho}_0\hat{U}^\dagger(t)e^{it(\hat{H}-\hat{V})}] = \text{tr}[e^{it\hat{H}_S}\hat{O}e^{-it\hat{H}_S}\hat{U}(t)\hat{\rho}_0\hat{U}^\dagger(t)] \quad (\text{A9})$$

and similarly

$$\text{tr}[\hat{O}e^{-it\hat{H}_L}\hat{\rho}_0e^{it\hat{H}_L}] = \text{tr}[e^{it\hat{H}_S}\hat{O}e^{-it\hat{H}_S}\hat{U}_L(t)\hat{\rho}_0\hat{U}_L^\dagger(t)]. \quad (\text{A10})$$

Hence,

$$\text{tr}[\hat{O}e^{-it\hat{H}}\hat{\rho}_0e^{it\hat{H}}] - \text{tr}[\hat{O}e^{-it\hat{H}_L}\hat{\rho}_0e^{it\hat{H}_L}] = \text{tr}[e^{it\hat{H}_S}\hat{O}e^{-it\hat{H}_S}(\hat{U}(t)\hat{\rho}_0\hat{U}^\dagger(t) - \hat{U}_L(t)\hat{\rho}_0\hat{U}_L^\dagger(t)) + [\hat{U}(t) - \hat{U}_L(t)]\hat{\rho}_0\hat{U}_L^\dagger(t)]. \quad (\text{A11})$$

Using the Cauchy-Schwarz inequality $|\text{tr}[\hat{A}\hat{B}\hat{\rho}_0]|^2 \leq \text{tr}[\hat{A}\hat{A}^\dagger\hat{\rho}_0]\text{tr}[\hat{B}^\dagger\hat{B}\hat{\rho}_0] \leq \|\hat{A}\|^2\text{tr}[\hat{B}^\dagger\hat{B}\hat{\rho}_0]$ and the triangle inequality, we find

$$\Delta(t, L) = |\text{tr}[\hat{O}e^{-it\hat{H}}\hat{\rho}_0e^{it\hat{H}}] - \text{tr}[\hat{O}e^{-it\hat{H}_L}\hat{\rho}_0e^{it\hat{H}_L}]| \leq 2\|\hat{O}\|\sqrt{\text{tr}[(\hat{U}^\dagger(t) - \hat{U}_L^\dagger(t))(\hat{U}(t) - \hat{U}_L(t))\hat{\rho}_0]}, \quad (\text{A12})$$

where

$$\text{tr}[(\hat{U}^\dagger(t) - \hat{U}_L^\dagger(t))(\hat{U}(t) - \hat{U}_L(t))\hat{\rho}_0] = -2\Re \int_0^t dx \frac{d}{dx} \text{tr}[\hat{U}^\dagger(x)\hat{U}_L(x)\hat{\rho}_0] \quad (\text{A13})$$

and

$$-i\frac{d}{dx}\hat{U}^\dagger(x)\hat{U}_L(x) = \hat{U}^\dagger(x)e^{ix\hat{H}_S}e^{ix\hat{H}_B}(\hat{V} - e^{-ix\hat{H}_B}e^{ix\hat{H}_B^L}\hat{V}e^{-ix\hat{H}_B^L}e^{ix\hat{H}_B})e^{-ix\hat{H}_B}e^{ix\hat{H}_B^L}e^{-ix\hat{H}_L}, \quad (\text{A14})$$

where

$$e^{-ix\hat{H}_B}e^{ix\hat{H}_B^L}\hat{V}e^{-ix\hat{H}_B^L}e^{ix\hat{H}_B} - \hat{V} = -i\hat{h} \int_0^x dy e^{-iy\hat{H}_B} [(\hat{H}_B - \hat{H}_B^L), e^{iy\hat{H}_B^L}\hat{x}_0e^{-iy\hat{H}_B^L}] e^{iy\hat{H}_B}. \quad (\text{A15})$$

Let us summarize the bound so far:

$$\frac{\Delta^2(t, L)}{8\|\hat{O}\|^2} \leq \int_0^t dx \int_0^x dy |\text{tr}[\hat{U}^\dagger(x)e^{ix\hat{H}_S}e^{ix\hat{H}_B}e^{-iy\hat{H}_B}\hat{h}[(\hat{H}_B - \hat{H}_B^L), e^{iy\hat{H}_B^L}\hat{x}_0e^{-iy\hat{H}_B^L}]e^{iy\hat{H}_B}e^{-ix\hat{H}_B}e^{ix\hat{H}_B^L}e^{-ix\hat{H}_L}\hat{\rho}_0]|. \quad (\text{A16})$$

We now proceed to bound the commutator and come back to Eq. (A16) after Eq. (A18). We have

$$\hat{H}_B - \hat{H}_B^L = \frac{1}{2} \sum_{i=L}^{\infty} \sum_{j=0}^{L-1} [\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j] + \frac{1}{2} \sum_{i=0}^{\infty} \sum_{j=L}^{\infty} [\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j] \quad (\text{A17})$$

such that, as only nearest neighbours are coupled and X and P are symmetric,

$$\begin{aligned} [(\hat{H}_B - \hat{H}_B^L), e^{iy\hat{H}_B^L}\hat{x}_0e^{-iy\hat{H}_B^L}] &= [\hat{x}_{L-1}, e^{iy\hat{H}_B^L}\hat{x}_0e^{-iy\hat{H}_B^L}] X_{L-1,L}\hat{x}_L + [\hat{p}_{L-1}, e^{iy\hat{H}_B^L}\hat{x}_0e^{-iy\hat{H}_B^L}] P_{L-1,L}\hat{p}_L \\ &=: C_{0,L-1}^{xx}(y)X_{L-1,L}\hat{x}_L + C_{0,L-1}^{xp}(y)P_{L-1,L}\hat{p}_L. \end{aligned} \quad (\text{A18})$$

Let us now come back to Eq. (A16). Inserting the above expression, we see that we need to bound terms of the form

$$F_r(x, y) = |\text{tr}[\hat{U}^\dagger(x)e^{ix\hat{H}_S}e^{ix\hat{H}_B}e^{-iy\hat{H}_B}\hat{h}\hat{r}_L e^{iy\hat{H}_B}e^{-ix\hat{H}_B}e^{ix\hat{H}_B^L}e^{-ix\hat{H}_L}\hat{\rho}_0]|. \quad (\text{A19})$$

with $r = x, p$. Writing $\hat{r}_L(t) = e^{it\hat{H}_B}\hat{r}_Le^{-it\hat{H}_B}$, $\hat{\rho}(x) = e^{ix(\hat{H}_L-\hat{V})}e^{-ix\hat{H}_L}\hat{\rho}_0e^{ix\hat{H}_L}e^{-ix(\hat{H}_L-\hat{V})}$, inserting the definition of $\hat{U}(x)$, and using $[\hat{H}_S, \hat{H}_B] = [\hat{H}_S, \hat{H}_B^L] = [\hat{H}_S, \hat{r}_L(t)] = 0$, this reads

$$F_r(x, y) = |\text{tr}[e^{ix(\hat{H}_L-\hat{V})}e^{-ix\hat{H}_L}e^{ix\hat{H}}\hat{h}e^{-ix\hat{H}_S}e^{-ix\hat{H}_B}\hat{r}_L(x-y)\hat{\rho}(x)]| \leq \|\hat{h}\|\sqrt{\text{tr}[\hat{r}_L^2(x-y)\hat{\rho}(x)]}, \quad (\text{A20})$$

where we used $|\text{tr}[\hat{A}\hat{B}\hat{\rho}(x)]|^2 \leq \|\hat{A}\|^2 \text{tr}[\hat{B}^\dagger \hat{B}\hat{\rho}(x)]$ to obtain the second line. Inserting Eqs. (A18,A20) into Eq. (A16), we hence have

$$\frac{\Delta^2(t, L)}{8\|\hat{O}\|^2\|\hat{h}\|} \leq |X_{L-1, L}| \int_0^t dx \int_0^x dy C_{0, L-1}^{xx}(x-y) \gamma_x(x, y) + |P_{L-1, L}| \int_0^t dx \int_0^x dy C_{0, L-1}^{xp}(x-y) \gamma_p(x, y), \quad (\text{A21})$$

where we denoted

$$\gamma_r(x, y) = \sqrt{\text{tr}[\hat{r}_L^2(y) \hat{\rho}(x)]}. \quad (\text{A22})$$

To keep track of the case $P \propto \mathbb{1}$, we let $P_{i,j} = 0$ for $|i-j| > R$ with $R = 0, 1$. By Eq. (56) in Ref. [16] and as $\|X_L P_L\| = \|P_L X_L\|$ [25], we have

$$\begin{aligned} |C_{0, L-1}^{xx}(y)| &\leq \sum_{\substack{n=0 \\ L \leq (n+1)(1+R)}}^{\infty} \frac{|y|^{2n+1}}{(2n+1)!} \|P_L X_L\|^n \|P_L\| \\ |C_{0, L-1}^{xp}(y)| &\leq \sum_{\substack{n=0 \\ L \leq n(1+R)+1}}^{\infty} \frac{|y|^{2n}}{(2n)!} \|P_L X_L\|^n. \end{aligned} \quad (\text{A23})$$

Bounding the second moments $\gamma_r(x, y)$ in the following section, we return to Eq. (A21) in Section A 1 b to complete the proof.

a. Second moments

Recalling that $\hat{\rho}(x) = e^{ix(\hat{H}_L - \hat{V})} e^{-ix\hat{H}_L} \hat{\rho}_0 e^{ix\hat{H}_L} e^{-ix(\hat{H}_L - \hat{V})}$, we find ($r = x, y$)

$$\begin{aligned} -i \frac{\partial}{\partial x} \text{tr}[\hat{r}_L^2(y) \hat{\rho}(x)] &= \text{tr}[\hat{r}_L^2(y) [\hat{\rho}(x), e^{ix(\hat{H}_L - \hat{V})} \hat{V} e^{-ix(\hat{H}_L - \hat{V})}]] \\ &= \text{tr}[\hat{\rho}(x) e^{ix\hat{H}_S} \hat{h} e^{-ix\hat{H}_S} [e^{ix\hat{H}_B^L} \hat{x}_0 e^{-ix\hat{H}_B^L}, \hat{r}_L^2(y)]] \\ &= 2 \text{tr}[\hat{\rho}(x) e^{ix\hat{H}_S} \hat{h} e^{-ix\hat{H}_S} [e^{ix\hat{H}_B^L} \hat{x}_0 e^{-ix\hat{H}_B^L}, \hat{r}_L(y)] \hat{r}_L(y)]. \end{aligned} \quad (\text{A24})$$

Now,

$$\hat{r}_k(y) = e^{iy\hat{H}_B} \hat{r}_k e^{-iy\hat{H}_B} = \sum_l c_{k,l}^{rx}(y) \hat{x}_l + \sum_l c_{k,l}^{rp}(y) \hat{p}_l, \quad (\text{A25})$$

where $r = x, y$ and

$$\begin{pmatrix} c_{xx}(y) & c_{xp}(y) \\ c_{px}(y) & c_{pp}(y) \end{pmatrix} = e^{-\sigma H_B y}, \quad H_B = X \oplus P, \quad \sigma = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}. \quad (\text{A26})$$

Hence,

$$\begin{aligned} -i \frac{\partial}{\partial x} \text{tr}[\hat{r}_L^2(y) \hat{\rho}(x)] &= 2 \text{tr}[\hat{\rho}(x) e^{ix\hat{H}_S} \hat{h} e^{-ix\hat{H}_S} \hat{r}_L(y)] \sum_{l=0}^{L-1} \left([e^{ix\hat{H}_B^L} \hat{x}_0 e^{-ix\hat{H}_B^L}, c_{L,l}^{rx}(y) \hat{x}_l + c_{L,l}^{rp}(y) \hat{p}_l] \right) \\ &= 2i \text{tr}[\hat{\rho}(x) e^{ix\hat{H}_S} \hat{h} e^{-ix\hat{H}_S} \hat{r}_L(y)] \sum_{l=0}^{L-1} \left(c_{L,l}^{rp}(y) d_{0,l}^{xx}(x) - c_{L,l}^{rx}(y) d_{0,l}^{xp}(x) \right), \end{aligned} \quad (\text{A27})$$

where

$$\begin{pmatrix} d_{xx}(x) & d_{xp}(x) \\ d_{px}(x) & d_{pp}(x) \end{pmatrix} = e^{-\sigma_L H_B^L x}, \quad H_B^L = X_L \oplus P_L, \quad \sigma_L = \begin{pmatrix} 0 & -\mathbb{1}_L \\ \mathbb{1}_L & 0 \end{pmatrix}. \quad (\text{A28})$$

We find

$$e^{-\sigma H_B y} \sigma \left[\begin{pmatrix} \mathbb{1}_L & 0 \\ 0 & 0 \\ 0 & \mathbb{1}_L \\ 0 & 0 \end{pmatrix} e^{-\sigma_L H_B^L x} \begin{pmatrix} \mathbb{1}_L & 0 & 0 & 0 \\ 0 & 0 & \mathbb{1}_L & 0 \end{pmatrix} \right]^t = \begin{pmatrix} c_{xp}(y) \begin{pmatrix} d_{xx}^t(x) & 0 \\ 0 & 0 \end{pmatrix} - c_{xx}(y) \begin{pmatrix} d_{xp}^t(x) & 0 \\ 0 & 0 \end{pmatrix} & * \\ c_{pp}(y) \begin{pmatrix} d_{xx}^t(x) & 0 \\ 0 & 0 \end{pmatrix} - c_{px}(y) \begin{pmatrix} d_{xp}^t(x) & 0 \\ 0 & 0 \end{pmatrix} & * \end{pmatrix}, \quad (\text{A29})$$

the operator norm (and therefore the absolute value of all entries) of which is upper bounded by $\|e^{H_B \sigma y}\| \|e^{H_B^L \sigma_L x}\|$. Therefore, employing $|\text{tr}[\hat{A} \hat{B} \hat{\rho}(x)]|^2 \leq \|\hat{A}\|^2 \text{tr}[\hat{B}^\dagger \hat{B} \hat{\rho}(x)]$,

$$\left| \frac{\partial}{\partial x} \text{tr}[\hat{r}_L^2(y) \hat{\rho}(x)] \right| \leq 2 \|e^{H_B \sigma y}\| \|e^{H_B^L \sigma_L x}\| \text{tr}[\hat{\rho}(x) e^{ix \hat{H}_S} \hat{h} e^{-ix \hat{H}_S} \hat{r}_L(y)] \leq 2 \|e^{H_B \sigma y}\| \|e^{H_B^L \sigma_L x}\| \|\hat{h}\| \sqrt{\text{tr}[\hat{\rho}(x) \hat{r}_L^2(y)]}, \quad (\text{A30})$$

which implies

$$\gamma_r(x, y) \leq \sqrt{\text{tr}[\hat{r}_L^2(y) \hat{\rho}_0]} + \|\hat{h}\| \|e^{H_B \sigma y}\| \int_0^x dz \|e^{H_B^L \sigma_L z}\|. \quad (\text{A36})$$

From Eq. (A25), we have, denoting $[\gamma_{xx}(y)]_{i,j} = \text{tr}[\hat{x}_i(y) \hat{x}_j(y) \hat{\rho}_0]$, $[\gamma_{xp}(y)]_{i,j} = \text{tr}[\hat{x}_i(y) \hat{p}_j(y) \hat{\rho}_0]$, $[\gamma_{px}(y)]_{i,j} = \text{tr}[\hat{p}_i(y) \hat{x}_j(y) \hat{\rho}_0]$, $[\gamma_{pp}(y)]_{i,j} = \text{tr}[\hat{p}_i(y) \hat{p}_j(y) \hat{\rho}_0]$,

$$\begin{pmatrix} \gamma_{xx}(y) & \gamma_{xp}(y) \\ \gamma_{px}(y) & \gamma_{pp}(y) \end{pmatrix} = e^{-\sigma H_B y} \gamma_0 (e^{-\sigma H_B y})^t, \quad (\text{A37})$$

i.e., all entries are bounded from above by $\|\gamma_0\| \|e^{H_B \sigma y}\|^2$, in particular $[\gamma_{rr}(y)]_{L,L}$ such that

$$\gamma_r(x, y) \leq \|\gamma_0\|^{1/2} \|e^{H_B \sigma y}\| + \|\hat{h}\| \|e^{H_B \sigma y}\| \int_0^x dz \|e^{H_B^L \sigma_L z}\|. \quad (\text{A38})$$

If $H_B > 0$, we may use the Williamson normal form to write $H_B \sigma = S^t (D \oplus D) S \sigma y = S^t (D \oplus D) \sigma (S^t)^{-1} y$, where $(D \oplus D) \sigma$ is real skew-symmetric, i.e., its eigenvalues are purely imaginary. Hence, $\|e^{H_B \sigma y}\| = \|e^{(D \oplus D) \sigma y}\| = 1$. We also have $\|e^{H_B \sigma y}\| = 1$ if $X = P$ as then σH_B is real skew-symmetric. Hence, c' an upper bound to $\max\{\|X\|, \|P\|\}$, we have

$$\gamma_r(x, y) \leq \begin{cases} \|\gamma_0\|^{1/2} + \|\hat{h}\| x & \text{if } X, P > 0 \text{ or } X = P, \\ \|\gamma_0\|^{1/2} e^{c' |y|} + \|\hat{h}\| e^{c' |y|} \frac{e^{c' x} - 1}{c'} & \text{otherwise,} \end{cases} \quad (\text{A39})$$

$$=: \gamma(x, y).$$

b. Final steps

Inserting the bounds in Eq. (A23) and Eq. (A39) into Eq. (A21) and letting c such that $\sqrt{\|P_L X_L\|} \leq c$, we have

$$\frac{\Delta^2(t, L)}{8 \|\hat{O}\|^2 \|\hat{h}\|} \leq \int_0^t dx \int_0^x dy \gamma(x, x-y) \left(\frac{\|P_L\| \|X_{L-1,L}\|}{c} \sum_{n=\lceil \frac{L}{1+R} \rceil}^{\infty} \frac{(cy)^{2n-1}}{(2n-1)!} + |P_{L-1,L}| \sum_{n=\lceil \frac{L-1}{2} \rceil}^{\infty} \frac{(cy)^{2n}}{(2n)!} \right), \quad (\text{A40})$$

where

$$\begin{aligned} \int_0^t dx \int_0^x dy \gamma(x, x-y) y^n &= \|\gamma_0\|^{1/2} \int_0^t dx \int_0^x dy e^{c'(x-y)} y^n + \|\hat{h}\| \int_0^t dx \int_0^x dy e^{c'(x-y)} \frac{e^{c'x} - 1}{c'} y^n \\ &\leq \frac{t^{n+2}}{(n+1)(n+2)} \left(\|\gamma_0\|^{1/2} + \|\hat{h}\| \frac{e^{c't} - 1}{c'} \right) e^{c't} \end{aligned} \quad (\text{A41})$$

and we may take $c' \rightarrow 0$ if $X, P > 0$ or $X = P$. For L even (odd) we have $\lceil \frac{L}{2} \rceil = L/2$ ($\lceil \frac{L}{2} \rceil = \frac{L+1}{2}$) and $\lceil \frac{L-1}{2} \rceil = L/2$ ($\lceil \frac{L-1}{2} \rceil = \frac{L-1}{2}$). Hence, for $R = 1$ the bound in the theorem follows. Finally, for $P \propto \mathbb{1}$ the second term in Eq. (A40) vanishes and we have $R = 0$.

Suppose

$$\left| \frac{d}{dx} \alpha(x) \right| \leq f(x) \sqrt{\alpha(x)} \quad (\text{A31})$$

and let $\alpha(0) = \alpha_0 \geq 0$. Then

$$\alpha(x) = \alpha_0 + \int_0^x dy \frac{d}{dy} \alpha(y) \leq \alpha_0 + \int_0^x dy f(y) \sqrt{\alpha(y)} =: \beta(x). \quad (\text{A32})$$

Let $\epsilon > 0$ and define $\gamma(x) = \beta(x) + \epsilon$. Then $\gamma(x) \geq \gamma(0) = \alpha_0 + \epsilon > 0$, i.e., $\sqrt{\gamma}$ is differentiable and

$$\sqrt{\beta(x) + \epsilon} = \sqrt{\gamma(x)} = \sqrt{\alpha_0 + \epsilon} + \int_0^x dy \frac{d}{dy} \sqrt{\gamma(y)}, \quad (\text{A33})$$

where

$$\int_0^x dy \frac{d}{dy} \sqrt{\gamma(y)} = \frac{1}{2} \int_0^x dy \frac{f(y) \sqrt{\alpha(y)}}{\sqrt{\gamma(y)}} \leq \frac{1}{2} \int_0^x dy f(y). \quad (\text{A34})$$

As $\epsilon > 0$ was arbitrary, we hence have

$$\sqrt{\alpha(x)} \leq \sqrt{\alpha_0} + \frac{1}{2} \int_0^x dy f(y). \quad (\text{A35})$$

c. Correlation matrix

The upper bound on the correlations $\gamma_{ab}(y)$, $a, b \in \{x, p\}$, in Eq. (A38) may be altered to allow for divergences at infinity by recalling that (see Eqs. (A25, A37))

$$\begin{pmatrix} \gamma_{xx}(y) & \gamma_{xp}(y) \\ \gamma_{px}(y) & \gamma_{pp}(y) \end{pmatrix} = e^{-\sigma H_B y} \gamma_0 (e^{-\sigma H_B y})^t = \begin{pmatrix} c_{xx}(y) & c_{xp}(y) \\ c_{px}(y) & c_{pp}(y) \end{pmatrix} \gamma_0 \begin{pmatrix} c_{xx}^t(y) & c_{px}^t(y) \\ c_{xp}^t(y) & c_{pp}^t(y) \end{pmatrix}, \quad (\text{A42})$$

i.e. (see Eq. (A37)),

$$\begin{aligned} \gamma_{xx}(y) &= c_{xx}(y)[\gamma_{xx}(0)c_{xx}^t(y) + \gamma_{xp}(0)c_{xp}^t(y)] + c_{xp}(y)[\gamma_{px}(0)c_{xx}^t(y) + \gamma_{pp}(0)c_{xp}^t(y)], \\ \gamma_{pp}(y) &= c_{px}(y)[\gamma_{xx}(0)c_{px}^t(y) + \gamma_{xp}(0)c_{pp}^t(y)] + c_{pp}(y)[\gamma_{px}(0)c_{px}^t(y) + \gamma_{pp}(0)c_{pp}^t(y)], \end{aligned} \quad (\text{A43})$$

and again using the bounds obtained in [16] which, however, increases the value of c in the bound.

d. Multiple baths

For some applications in quantum biology and condensed matter physics, one has a quantum system coupled to N baths which, using the Particle or Phonon mapping, can be written in the form

$$\hat{H}^{mul.} = \hat{H}_S + \sum_{m=1}^N \hat{H}^{(m)} + \sum_{m=1}^N \hat{h}^{(m)} \hat{x}_0^{(m)} \quad (\text{A44})$$

where

$$\hat{H}^{(m)} = \frac{1}{2} \sum_{i,j=0}^{\infty} [\hat{x}_i^{(m)} X_{i,j}^{(m)} \hat{x}_j^{(m)} + \hat{p}_i^{(m)} P_{i,j}^{(m)} \hat{p}_j^{(m)}], \quad (\text{A45})$$

and $X_{i,j}^{(m)} = X_{j,i}^{(m)} \in \mathbb{R}$, $P_{i,j}^{(m)} = P_{j,i}^{(m)} \in \mathbb{R}$. As in the rest of this work so far we assume that they couple only nearest neighbours, i.e. $X_{i,j}^{(m)} = P_{i,j}^{(m)} = 0$ for $|i - j| > 1$. We can truncate the N chains such that the m^{th} chain contains L_m modes:

$$\hat{H}_L^{mul.} = \hat{H}_S + \sum_{m=1}^N \hat{H}_{L_m}^{(m)} + \sum_{m=1}^N \hat{h}^{(m)} \hat{x}_0^{(m)}, \quad (\text{A46})$$

where

$$\hat{H}_{L_m}^{(m)} = \frac{1}{2} \sum_{i,j=0}^{L_m-1} [\hat{x}_i^{(m)} X_{i,j}^{(m)} \hat{x}_j^{(m)} + \hat{p}_i^{(m)} P_{i,j}^{(m)} \hat{p}_j^{(m)}] = \frac{1}{2} \sum_{i,j} [\hat{x}_i^{(m)} (X_{L_m})_{i,j} \hat{x}_j^{(m)} + \hat{p}_i^{(m)} (P_{L_m})_{i,j} \hat{p}_j^{(m)}], \quad (\text{A47})$$

where X_{L_m} and P_{L_m} are principle submatrices of $X^{(m)}$ and $P^{(m)}$ corresponding to the non-truncated modes. These definitions are in analogy with those at the beginning of section A but generalised to the case of N non identical copies of the bath.

Corollary 1 (Multiple chains) Let $\hat{H}^{mul.}$, $\hat{H}_L^{mul.}$ as above, c_m, c'_m such that $\|P_{L_m} X_{L_m}\|^{1/2} \leq c_m$ and $\max \{\|X^{(m)}\|, \|P^{(m)}\|\} \leq c'_m$. Then the error in truncating $\hat{H}^{mul.}$ by $\hat{H}_L^{mul.}$ is bounded by

$$\Delta(L, t) := |\text{tr}[\hat{O} e^{-i\hat{H}^{mul.}t} \hat{\rho}_0 e^{i\hat{H}^{mul.}t}] - \text{tr}[\hat{O} e^{-i\hat{H}_L^{mul.}t} \hat{\rho}_0 e^{i\hat{H}_L^{mul.}t}]| \leq \sum_{m=1}^N F(m, t, L_m) \quad (\text{A48})$$

where we have defined $F \geq 0$ as

$$F^2(m, t, L) := 4\|\hat{O}\|^2 \frac{\|\hat{h}^{(m)}\|}{c_m} \left(\frac{\|P_L\| \|X_{L-1,L}^{(m)}\|}{c_m^2} + \frac{|P_{L-1,L}^{(m)}|}{c_m} \right) \frac{(c_m t)^{L+1}}{(L+1)!} (e^{c_m t} + 1) \left(\|\gamma_0^{(m)}\|^{1/2} + \|\hat{h}^{(m)}\| \frac{e^{c'_m t} - 1}{c'_m} \right) e^{c'_m t}. \quad (\text{A49})$$

If $X^{(m)}, P^{(m)} > 0$ or $X^{(m)} = P^{(m)}$, we may take $c'_m \rightarrow 0$. If $P^{(m)} \propto \mathbb{1}$, we may replace $\frac{(c_m t)^{1+L_m}}{(L_m+1)!}$ by $\frac{(c_m t)^{2L_m+1}}{(2L_m+1)!}$. Here,

$$\gamma_0^{(m)} = \begin{pmatrix} \gamma_{xx}^{(m)} & \gamma_{xp}^{(m)} \\ \gamma_{xp}^{(m)\dagger} & \gamma_{pp}^{(m)} \end{pmatrix}, \quad [\gamma_{xx}^{(m)}]_{i,j} = \text{tr}[\hat{x}_i^{(m)} \hat{x}_j^{(m)} \hat{\rho}_0], \quad [\gamma_{pp}^{(m)}]_{i,j} = \text{tr}[\hat{p}_i^{(m)} \hat{p}_j^{(m)} \hat{\rho}_0], \quad [\gamma_{xp}^{(m)}]_{i,j} = \text{tr}[\hat{x}_i^{(m)} \hat{p}_j^{(m)} \hat{\rho}_0], \quad (\text{A50})$$

collects the two-point m^{th} bath correlations in the initial state of the whole system. Note that $\|X_{L_m}^{(m)}\| \leq \|X^{(m)}\|$ and $\|P_{L_m}^{(m)}\| \leq \|P^{(m)}\|$.

As with theorem 2, one can allow for the two-point correlations collected in $\gamma_0^{(m)}$ to diverge and still get a bound on F , see Section A 1 c. Often, one encounters systems interacting with multiple baths. We generalize to this setting in Section A 1 d.

Proof. Starting from

$$\text{tr}[\hat{O}e^{-i\hat{H}^{\text{mul}}t}\hat{\rho}_0e^{i\hat{H}^{\text{mul}}t}] - \text{tr}[\hat{O}e^{-i\hat{H}_L^{\text{mul}}t}\hat{\rho}_0e^{i\hat{H}_L^{\text{mul}}t}], \quad (\text{A51})$$

we add and subtract

$$\text{tr}[\hat{O}e^{-i\hat{H}_{tru}t}\hat{\rho}_0e^{i\hat{H}_{tru}t}] \quad (\text{A52})$$

$N - 1$ times where \hat{H}_{tru} corresponds to H^{mul} but with some of the N baths truncated. Each time it is added and subtracted, different baths should be truncated. We then group the terms in pairs of 2 and redefine the system in each pair such that the system contains $N - 1$ baths (some truncated, some not). This step relies crucially on the fact that the system Hamiltonian \hat{H}_s is not necessarily bounded. We then take the absolute value and apply the triangle inequality to the pairs followed by applying theorem 1 to each pair. \square

Thus the error introduced by truncating N chains, is bounded by the sum of the errors of truncating each chain individually. The explicit forms of the bound for the Particle and Phonon mapping can be found in section B.

Appendix B: Derivation of the particle and phonon mapping chain truncation bounds

From [9] we find Particle and Phonon mappings of Eq. (7) to be

$$\hat{H} = \hat{H}_S + \sqrt{\beta_0(0)}\hat{A}_S(b_0(0) + b_0^\dagger(0)) + \sum_{n=0}^{\infty} \left(\alpha_n(0)b_n^\dagger(0)b_n(0) + \sqrt{\beta_{n+1}(0)}(b_{n+1}^\dagger(0)b_n(0) + h.c.) \right) \quad (\text{B1})$$

and

$$\hat{H} = \hat{H}_S + \sqrt{\beta_0(1)}\hat{A}_S\hat{x}_0(1) + \sum_{n=0}^{\infty} \left(\frac{\alpha_n(1)}{2}\hat{x}_n^2(1) + \frac{1}{2}\hat{p}_n^2(1) + \sqrt{\beta_{n+1}(1)}\hat{x}_n(1)\hat{x}_{n+1}(1) \right), \quad (\text{B2})$$

respectively. $b_n^\dagger(0)$, $(b_n(0))$, are creation (annihilation) operators. Define position and momentum operators for the particle mapping $\hat{x}_n(0) := (b_n^\dagger(0) + b_n(0))/\sqrt{2}$, $\hat{p}_n(0) := i(b_n^\dagger(0) - b_n(0))/\sqrt{2}$ and $\hat{x}_n(1) := \sqrt{\omega_{max}}\hat{x}_n(1)$, $\hat{p}_n(1) := \hat{p}_n(1)/\sqrt{\omega_{max}}$ for the phonon mapping. Write Eqs. (B1), (B2) in terms of these new operators and compare these Eqs. with Eqs. (2) and (1). From here, together with the definition of the Jacobi matrices $\mathcal{J}(d\lambda^q)$ (see Eq. (162) in [9]), we find:

For the particle mapping

$$X = P = \mathcal{J}(d\lambda^0), \quad \hat{h} = \sqrt{2\beta_0(0)}\hat{A}_S, \quad d\lambda^0(x) = J(x)dx/\pi. \quad (\text{B3})$$

For the phonon mapping

$$X = \frac{\mathcal{J}(d\lambda^1)}{\omega_{max}}, \quad P = \mathbb{1} \omega_{max}, \quad \hat{h} = \sqrt{\frac{\beta_0(1)}{\omega_{max}}}\hat{A}_S, \quad d\lambda^1(x) = J(\sqrt{x})dx/\pi. \quad (\text{B4})$$

From Eqs (15,156,160) in [9],

$$\beta_0(0) = \int_{\omega_{min}}^{\omega_{max}} dx J(x)/\pi, \quad \beta_0(1) = \int_{\omega_{min}^2}^{\omega_{max}^2} dx J(\sqrt{x})/\pi. \quad (\text{B5})$$

Since the spectrum of a Jacobi matrix is equal to its minimally closed support interval [26], we have for the particle and phonon mappings: $\|X\| = \|P\| = \sqrt{\|XP\|} = \omega_{max}$, and $X > 0$ iff $\omega_{min} > 0$. For the Particle mapping we can use Eq. (A6) with $c = c' = \omega_{max}$ to achieve

$$\Delta^2(t, L) \leq 8\mu_0 \|\hat{O}\|^2 \frac{\|\hat{A}_S\| (\omega_{max}t)^{L+1}}{\omega_{max} (L+1)!} (e^{\omega_{max}t} + 1) \left(\|\gamma_0\|^{1/2} + \mu_0 \|\hat{A}_S\|t \right) \quad (\text{B6})$$

where μ_0 given by Eq. (11). For the massive Phonon mapping, we replace 8 with 4, μ_0 with μ_1 , and $(\omega_{max}t)^{L+1}/(L+1)!$ by $(\omega_{max}t)^{2L+1}/(2L+1)!$ in Eq. (B6). For the massless Phonon chain mapping, we use Eq. (A6) again, to achieve

$$\Delta^2(t, L) \leq 4\mu_1 \|\hat{O}\|^2 \frac{\|\hat{A}_S\| (\omega_{max}t)^{2L+1}}{\omega_{max} (2L+1)!} (e^{\omega_{max}t} + 1) \left(\|\gamma_0\|^{1/2} + \|\hat{h}\| \frac{e^{\omega_{max}t} - 1}{\omega_{max}} \right) e^{\omega_{max}t}. \quad (B7)$$

We can write the γ_0 matrix for the Phonon mapping in terms of the original \hat{x}_n and \hat{p}_n coordinates of Eq. 10, to find

$$\gamma_0 = \begin{pmatrix} \omega_{max}\gamma_{xx} & \gamma_{xp} \\ \gamma_{px} & \frac{1}{\omega_{max}}\gamma_{pp} \end{pmatrix}, \quad [\gamma_{ab}]_{n,l} = \text{tr}[\hat{a}_n \hat{b}_l \hat{\rho}_0]. \quad (B8)$$

Appendix C: Fock space truncation

In this section we derive bounds on the error introduced by truncating the local Hilbert spaces of the bath. To this end, we define the projector

$$\mathbb{1}_{\mathbf{m}} = \mathbb{1}_{m_0} \otimes \mathbb{1}_{m_1} \otimes \cdots, \quad (C1)$$

where $\mathbb{1}_{m_i}$ acts on the i 'th site of the bath and truncates the local Hilbert space according to

$$\mathbb{1}_m = \sum_{n=0}^m |n\rangle\langle n|. \quad (C2)$$

For bounded observables acting on the system \hat{O} , $\|\hat{O}\| < \infty$, we consider

$$\Delta_{\mathbf{m}}(t) = |\text{tr}[\hat{O}e^{-it\hat{H}}\hat{\rho}_0e^{it\hat{H}}] - \text{tr}[\hat{O}e^{-it\hat{H}_{\mathbf{m}}}\hat{\rho}_0e^{it\hat{H}_{\mathbf{m}}}]|, \quad (C3)$$

i.e., the error introduced by evolving the system according to

$$\hat{H}_{\mathbf{m}} = \mathbb{1}_{\mathbf{m}}\hat{H}\mathbb{1}_{\mathbf{m}} = \hat{H}_S + \hat{H}_B^{\mathbf{m}} + \hat{V}_{\mathbf{m}} \quad (C4)$$

instead of $\hat{H} = \hat{H}_S + \hat{H}_B + \hat{V}$. Here, with the notation $\hat{x}_i^{\mathbf{m}} = \mathbb{1}_{\mathbf{m}}\hat{x}_i\mathbb{1}_{\mathbf{m}}$ and $\hat{p}_i^{\mathbf{m}} = \mathbb{1}_{\mathbf{m}}\hat{p}_i\mathbb{1}_{\mathbf{m}}$, the individual terms read $\hat{V}_{\mathbf{m}} = \hat{h} \otimes \hat{x}_0^{\mathbf{m}}$ and

$$\hat{H}_B^{\mathbf{m}} = \mathbb{1}_{\mathbf{m}}\hat{H}_B\mathbb{1}_{\mathbf{m}} = \frac{1}{2} \sum_{i,j} [X_{i,j}\mathbb{1}_{\mathbf{m}}\hat{x}_i\hat{x}_j\mathbb{1}_{\mathbf{m}} + P_{i,j}\mathbb{1}_{\mathbf{m}}\hat{p}_i\hat{p}_j\mathbb{1}_{\mathbf{m}}], \quad (C5)$$

where we note that $\mathbb{1}_{\mathbf{m}}\hat{x}_i^2\mathbb{1}_{\mathbf{m}} \neq (\hat{x}_i^{\mathbf{m}})^2$ and $\mathbb{1}_{\mathbf{m}}\hat{p}_i^2\mathbb{1}_{\mathbf{m}} \neq (\hat{p}_i^{\mathbf{m}})^2$, while for $i \neq j$ we do have $\mathbb{1}_{\mathbf{m}}\hat{x}_i\hat{x}_j\mathbb{1}_{\mathbf{m}} = \hat{x}_i^{\mathbf{m}}\hat{x}_j^{\mathbf{m}}$ and $\mathbb{1}_{\mathbf{m}}\hat{p}_i\hat{p}_j\mathbb{1}_{\mathbf{m}} = \hat{p}_i^{\mathbf{m}}\hat{p}_j^{\mathbf{m}}$. Now denote

$$\begin{aligned} \hat{U}(t) &= e^{it(\hat{H}-\hat{V})}e^{-it\hat{H}}, \\ \hat{U}_{\mathbf{m}}(t) &= e^{it(\hat{H}_{\mathbf{m}}-\hat{V}_{\mathbf{m}})}e^{-it\hat{H}_{\mathbf{m}}}. \end{aligned} \quad (C6)$$

Proceeding as in Eqs. (A9-A12), we find

$$\Delta_{\mathbf{m}}(t) = |\text{tr}[\hat{O}e^{-it\hat{H}}\hat{\rho}_0e^{it\hat{H}}] - \text{tr}[\hat{O}e^{-it\hat{H}_{\mathbf{m}}}\hat{\rho}_0e^{it\hat{H}_{\mathbf{m}}}]| \leq 2\|\hat{O}\| \sqrt{\text{tr}[(\hat{U}^\dagger(t) - \hat{U}_{\mathbf{m}}^\dagger(t))(\hat{U}(t) - \hat{U}_{\mathbf{m}}(t))\hat{\rho}_0]}, \quad (C7)$$

where now, as $\hat{U}_{\mathbf{m}}^\dagger(t)\hat{U}_{\mathbf{m}}(t) = \mathbb{1}_S \otimes \mathbb{1}_{\mathbf{m}}$,

$$\text{tr}[(\hat{U}^\dagger(t) - \hat{U}_{\mathbf{m}}^\dagger(t))(\hat{U}(t) - \hat{U}_{\mathbf{m}}(t))\hat{\rho}_0] = \text{tr}[(\mathbb{1} - \mathbb{1}_{\mathbf{m}})\hat{\rho}_0] - 2\Re \int_0^t dx \frac{d}{dx} \text{tr}[\hat{U}^\dagger(x)\hat{U}_{\mathbf{m}}(x)\hat{\rho}_0] \quad (C8)$$

and

$$\begin{aligned} -i \frac{d}{dx} \hat{U}^\dagger(x)\hat{U}_{\mathbf{m}}(x) &= \hat{U}^\dagger(x)e^{ix\hat{H}_S}\hat{h}(e^{ix\hat{H}_B}\hat{x}_0e^{-ix\hat{H}_B} - e^{ix\hat{H}_B^{\mathbf{m}}}\hat{x}_0e^{-ix\hat{H}_B^{\mathbf{m}}})e^{ix\hat{H}_B^{\mathbf{m}}}e^{-ix\hat{H}_{\mathbf{m}}} \\ &=: \hat{U}^\dagger(x)e^{ix\hat{H}_S}\hat{h}\hat{W}(x)e^{ix\hat{H}_B^{\mathbf{m}}}e^{-ix\hat{H}_{\mathbf{m}}}. \end{aligned} \quad (C9)$$

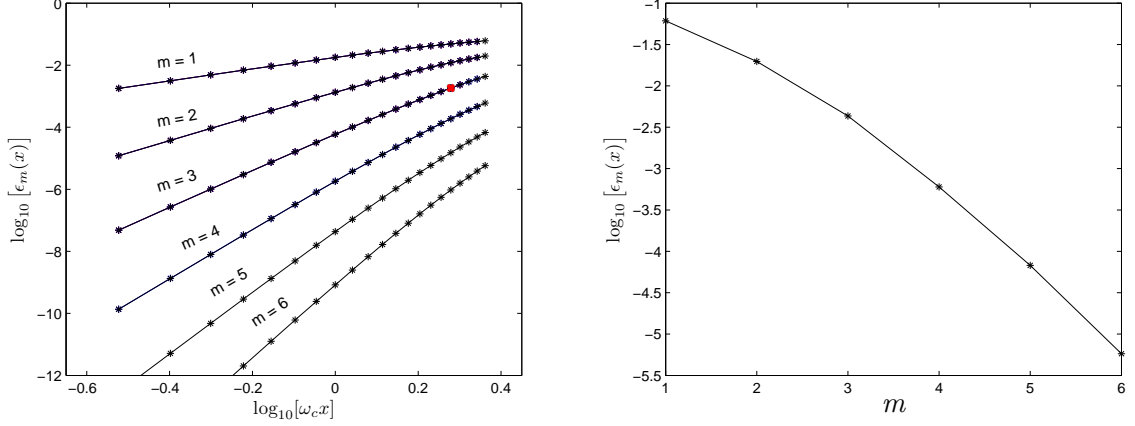


FIG. 3. Fock space truncation error (Eq. (17)) for the model in Eq. (19) using the particle mapping with $\Delta/\omega_c = 1$, $\alpha = 0.8$, $s = 1$ for initial state $\hat{\rho}_0 = \hat{\rho}_S^0 \otimes \hat{\rho}_B^0$, $\hat{\rho}_S^0 = |\uparrow\rangle\langle\uparrow|$ and $\hat{\rho}_B^0$ the vacuum. We truncate each local Hilbert space at the same value $m_i = m$ and L has the values 3 to 6, but are indistinguishable (e.g. the difference between the $L = 6$ and $L = 3$ curve at the point denoted by a square is 4.86×10^{-8}). Lines are guides to the eye.

The Cauchy–Schwarz inequality yields

$$\left| \frac{d}{dx} \text{tr} [\hat{U}^\dagger(x) \hat{U}_m(x) \hat{\rho}_0] \right|^2 \leq \text{tr} [\hat{h}^2 e^{-ix\hat{H}_B^m} \hat{W}^2(x) e^{ix\hat{H}_B^m} e^{-ix\hat{H}_m} \hat{\rho}_0 e^{ix\hat{H}_m}] =: \epsilon_m(x) \quad (\text{C10})$$

such that

$$\Delta_m^2(t) \leq 4 \|\hat{O}\|^2 \left(\text{tr}[(\mathbb{1} - \mathbb{1}_m) \hat{\rho}_0] + 2 \int_0^t dx \sqrt{\epsilon_m(x)} \right). \quad (\text{C11})$$

The error $\epsilon_m(x)$ may be obtained numerically: We have

$$\begin{aligned} e^{-ix\hat{H}_B^m} \hat{W}^2(x) e^{ix\hat{H}_B^m} &= e^{-ix\hat{H}_B^m} \hat{W}(x) \mathbb{1}_m \hat{W}(x) e^{ix\hat{H}_B^m} + e^{-ix\hat{H}_B^m} \hat{W}(x) (\mathbb{1} - \mathbb{1}_m) \hat{W}(x) e^{ix\hat{H}_B^m} \\ &= e^{-ix\hat{H}_B^m} (\hat{x}_0(x) - e^{ix\hat{H}_B^m} \hat{x}_0 e^{-ix\hat{H}_B^m}) \mathbb{1}_m (\hat{x}_0(x) - e^{ix\hat{H}_B^m} \hat{x}_0 e^{-ix\hat{H}_B^m}) e^{ix\hat{H}_B^m} \\ &\quad + e^{-ix\hat{H}_B^m} \hat{x}_0(x) (\mathbb{1} - \mathbb{1}_m) \hat{x}_0(x) e^{ix\hat{H}_B^m} \end{aligned} \quad (\text{C12})$$

such that, recalling Eq. (A25), i.e., that $\hat{x}_0(t) = e^{it\hat{H}_B} \hat{x}_0 e^{-it\hat{H}_B} = \sum_k c_{0,k}^{xx}(t) \hat{x}_k + \sum_k c_{0,k}^{xp}(t) \hat{p}_k$, the computation of $\epsilon_m(x)$ is reduced to obtaining the coefficients $c_{0,k}^{xx}(t)$ and $c_{0,k}^{xp}(t)$ and expectations in $e^{-ix\hat{H}_m} \hat{\rho}_0 e^{ix\hat{H}_m}$ of observables of the form

$$\hat{h}^2 \otimes (e^{-ix\hat{H}_B^m} \hat{r}_k^m e^{ix\hat{H}_B^m} - \hat{x}_0^m) (e^{-ix\hat{H}_B^m} \hat{s}_l^m e^{ix\hat{H}_B^m} - \hat{x}_0^m) \quad (\text{C13})$$

and

$$\hat{h}^2 \otimes \mathbb{1}_m \hat{r}_k (\mathbb{1} - \mathbb{1}_m) \hat{s}_l \mathbb{1}_m = \delta_{k,l} \hat{h}^2 \otimes \mathbb{1}_m \hat{r}_k (\mathbb{1} - \mathbb{1}_m) \hat{s}_k \mathbb{1}_m \quad (\text{C14})$$

for $r, s \in \{x, p\}$.

Appendix D: Further numerical examples of Fock space truncation

In this section, we give the chain coefficients used in the numerical simulations for the Fock space truncation and analyse further the numerical results. We start with the particle mapping of the spin-boson model: From Eq. (B3), we have the relation between the X and P matrices and the Jacobi matrix. The coefficients of the Jacobi matrix for the spin-boson spectral density

of Eq. (19) can be found in [7] or [9]. From Eqs. (248), (249) in [9], we have for $n \in \mathbb{N}^0$,

$$X_{n+1,n+1} = \frac{\omega_c}{2} \left(1 + \frac{s^2}{(s+2n)(2+s+2n)} \right), \quad (\text{D1})$$

$$X_{n,n+1} = X_{n+1,n} \quad (\text{D2})$$

$$= \frac{\omega_c(1+n)(1+s+n)}{(s+2+2n)(3+s+2n)} \sqrt{\frac{3+s+2n}{1+s+2n}}, \quad (\text{D3})$$

and all other matrix elements zero. $\beta_0(0)$ can be found in Eq. (250) in [9], thus from Eq. (B3), we have

$$\hat{h} = \omega_c \sqrt{\frac{2\alpha}{s+1}} \hat{A}_S. \quad (\text{D4})$$

We can now do the same for the phonon mapping written in terms of \hat{x}_n , and \hat{p}_n . Using Eq. (B4), we have the relation between the X and P matrices and the Jacobi matrix. From [9], we obtain the coefficients of the Jacobi matrix. Thus, using Eqs. (255), (256) in [9], we have for $n \in \mathbb{N}^0$,

$$X_{n+1,n+1} = \frac{\omega_c}{2} \left(1 + \frac{s^2}{(s+4n)(4+s+4n)} \right), \quad (\text{D5})$$

$$X_{n,n+1} = X_{n+1,n} = \frac{\omega_c 2(1+n)(2+s+2n)}{(s+4+4n)(6+s+4n)} \sqrt{\frac{6+s+4n}{2+s+4n}}, \quad (\text{D6})$$

and all other matrix elements zero. $\beta_0(1)$ can be found in Eq. (257) in [9], thus from Eq. (B4), we have

$$\hat{h} = \omega_c \sqrt{\frac{2\alpha}{s+2}} \hat{A}_S. \quad (\text{D7})$$

The results for the particle mapping with Ohmic spectral density are plotted in Fig. 3 and for the phonon mapping in Fig. 2. In both cases, the plots suggest that the super ohmic spectral densities have smaller truncation error. For the particle mappings, in the plots we have probed the zero Kelvin thermal state (which corresponds to the chain vacuum state), where as for the phonon mappings we have probed a squeezed vacuum state, which is highly populated. We see that the error has slightly worse decay with increasing m than in the particle mappings cases. This is intuitively what one would expect, since more of the bath population is being truncated.

We probed the vacuum state of the chain, which corresponds to a squeezed vacuum state of the continuous bath of harmonic oscillators. This will be

shown in an upcoming article [27].